 Manual by R.T. Oakley, July 1997. Updated by U.M. Oehler

User's Manual

Contents

Chapter 1 - Overview of the Hermes Suite

1.1 Introduction Windows 95 based word processors are large and powerful, with any number of options for formatting and printing both text and graphical material. As such they serve as excellent vehicles for desk-top publishing. They can, in conjunction with a variety of database programs, also provide excellent platforms for the preparation of program schedules and abstract books for conferences of all types. However, the flexibility of most word processors comes at a cost. If a very specific task is to be performed, on a regular basis, then the many options within most commercial word processing packages are at least redundant, and can even create problems. These difficulties are most apparent when conference organizers turn their minds to the idea of electronic submission of abstracts, a concept which, in principle, should considerably reduce the burden of processing the abstracts themselves and all the other data required for the generation of a conference program.

In essence the flexibility afforded by most word processors can inhibit rather than facilitate the preparation of documents where strict format and size control are vital. If a very specific task is to be performed, all that is needed is a simple, highly formatted word and data processor with full text and graphical editing capabilities. The Hermes Suite is a software package designed to meet these requirements. Its sole function is to facilitate the preparation, submission, scheduling and publication of papers and abstracts submitted to scientific conferences. The idea for such software was spawned from the experiences of the organizing committee of the 78th Canadian Society for Chemistry Conference held at the University of Guelph in June 1995. The Hermes Suite was initially designed to meet the organizational needs and format requirements of the Canadian Society for Chemistry (CSC). Any conference operating with guidelines similar to those used by the CSC can, in principle, take advantage of this software. The Suite consists of three main components, only one of which (Hermes, the electronic abstract) is distributed to the presenting authors. The other two (Charon and Tartarus) are used exclusively by the conference organizers for the receipt and scheduling of presentations. The current version of the Hermes Suite provides the following output for conference organizers:

1. The full conference program, formatted and indexed.

2. An complete abstract book, with either 6, 4, 2 or 1 abstract(s) per page according to the preferences of the conference organizers.

3. Fully formatted room signs.

4. Electronic (HTML) versions of the full conference program, along with downloadable versions (via Adobe Acrobat) of all conference abstracts (text and graphics).

The three components of the Hermes Suite are summarized below. Details of the function and operation of each are the subjects of subsequent chapters.

Hermes is a stand-alone word processor/form filler for the creation of scientific abstracts. It runs under Windows 2K, NT4, 98, 95 and Windows 3.1 (Win32S extension installed); *there is no MAC version*. In many ways Hermes resembles a typical Windows based word processor program (*e.g.*, WORD, WordPerfect). For example, Hermes allows the author to see, *via* preview mode or by printing hardcopy, *exactly* how his/her abstract will appear in the final abstract book and on the World Wide Web. However, in contrast to a normal word processor, in which a wide range of font and format control exists, the font and page size is predetermined by the conference organizers so that the length of the abstract *cannot* be changed by the user. Thus, both the author and the organizer will know exactly what the final abstract will look like. There is little or no need for later editing by conference organizers.

Hermes is also designed so that all the information necessary for the generation of the conference program and abstract book, *i.e.*, author names, addresses, symposium details, presentation format (poster/oral), are entered easily and quickly in a manner which allows automatic retrieval by the conference organizers from the electronic abstract. Graphical inserts, a common feature of many scientific abstracts, can also be incorporated from virtually any other Windows application *via* clipboard cut and paste. Once saved to disk, Hermes abstract files can be submitted by web-upload.

Charon Charon operates under Windows 95 or 98. It is a program for the receipt and processing of electronic abstracts prepared by Hermes. Charon is also used to define the conference structure, *e.g.*, the Divisions, Symposia, names of organizers, which are specific to any conference. Details on abstract submission (how, when and where) must also incorporated. This *initialization* procedure creates the database to be used during the abstract receipt stage. It also generates a blueprint or template (the so-called .HRM file) which must be distributed to users of Hermes, so that the abstract preparation program and the organizer's abstract receipt program map onto the same database.

Tartarus Tartarus also operates under Windows 95 or 98. Its function is to provide the program organizers with a means of scheduling papers into Divisions and Symposia. It also generates hardcopy versions of the Conference Program (fully formatted and indexed), the Abstract Book and all the necessary "signage" for rooms. Web versions of the program, schedule and abstract book are also prepared (as HTML and GIF files).

1.2 System Requirements

Hermes Minimum author requirements are a 486/66 with 8 MB RAM, operating under 3.1 (with WIN 32S extensions installed) or Windows 95.

Charon and Tartarus Conference organizers should minimally employ a fast Pentium III or Athlon system running Windows 95 or 98, with 64MB of RAM and a gigabyte of free hard drive space. The computer should have a reliable back-up device such as an Iomega Zip drive or a CDR or CDRW drive.

Printer The recommended (default) printer is an HP LaserJet 5P. Any high quality 600 dpi printer will, however, suffice. Subsequent duplication of hardcopy material is the responsibility of the conference organizers. Users may experience some minor format (margin and offset) problems with other printers, in which case contact O'Zone software.

E- Mail and Internet Connections The computer system used for Charon and Tartarus must be WINSOCK compliant and have access to an SMTP system. The World Wide Web documents and pages can be copied or FTP'd to any web server for distribution.

1.3 Installation of the Hermes Suite

The Hermes Suite will typically be supplied to you by O'Zone Software electronically via FTP. There will be two components.

A file called HSUITE.EXE, installs a generic version of the Hermes Suite. This will create a directory `c:\HSUITE` (this default location can be changed by the operator). A **Hermes Suite** program group will also be generated. It will contain program icons for Hermes, Charon and Tartarus.

A file called CHANGES.EXE will update the generic installation to one specific to your conference.

1.4 On-line Help Extensive on-line HELP on all aspects of software operation is provided within Hermes, Charon and Tartarus.

Chapter 2 - Charon

2.1 Introduction The main purpose of Charon is to allow conference organizers to enter information regarding each abstract submitted to the conference into a master database. Later, once all the abstracts are received, (or concurrently) this database will be used by Tartarus for the construction of the conference program. It is expected that most abstracts will be prepared using Hermes (either by the submitters or by conference staff) and the subsequent files read into Charon and stored in the database. It is also possible to prepare an abstract within Charon (from the keyboard) and then store the abstract in the database. Abstracts entered into the database by either mechanism can be edited at any time for style or content. Charon also contains an option for automatic notification of receipt, by e-mail, to the submitting author. However, before any abstract can be received and processed, the conference database into which all abstracts and related information will eventually be deposited must be assembled. This information, which is unique to the conference, will subsequently be transmitted to submitting authors in the form of a .HRM file. Once this file is loaded into Hermes, authors can enter the appropriate information as requested, and return the abstract in the manner prescribed.

2.2 Initialization of Charon

The initialization process will typically be performed by O'Zone Software using your call-for-papers and other related information. The customized files will be packaged as a CHANGES.EXE program which will be used by the conference organizers to convert their generic Hermes Suite installation into one specific to their conference. In principle, however, the initialization could also be done by the conference organizers.

2.2.1 Conference Data When Charon is loaded, by double clicking on the Charon ICON within Windows, the default screen presents the operator with the Conference Data folder. In a typical CSC-like Conference, all papers must be categorized by Division and Symposium. The default duration of oral presentations must be also specified, as well as the names of the symposium organizers. To this end, enter the following information into the appropriate screen locations. Note that this data will be used - as entered - at later points in the elaboration of the conference. Spelling mistakes and format features made here will reemerge later.

1. **Select Master Printer** When composing a document in your favourite word processor, changing the destination printer can change the points at which lines of text break. This occurs even though the same TrueType font is used in each case. When TrueType fonts are downloaded to different printers, the widths for any given letter (font metrics) can vary. This is what causes lines of text to break at different points.

Since the appearance of an abstract should be constant, regardless of the destination printer, the Hermes Suite uses the concept of a Master Printer. The letter widths of each font are recorded for one specific printer (the Master Printer). These letter widths are then used to override any given printer's natural letter spacing. This guarantees that text lines will break at reproducible points.

The default master printer for the conference program and abstracts is an HP LaserJet 4. Typically there is no need to change this setting as differences in letter spacing, while finite, are typically small. The small differences in letter spacing caused by using the Master Printer's metrics as opposed to those of the actual printer used to print are not normally visible. If a test print shows no problems then this setting should be left at it's default. If a test print shows objectionable anomalies in letter spacing, the Master Printer should be set to the actual output printer.

If the organizers wish to specify a different printer (a fast, high resolution - min 600 dpi - printer is recommended), the decision to change must be made *before* the .HRM file is generated. Invoking the option to change the printer will require that the appropriate Windows driver be loaded.

2. **Name of Conference** This should be self-explanatory, *e.g.*,

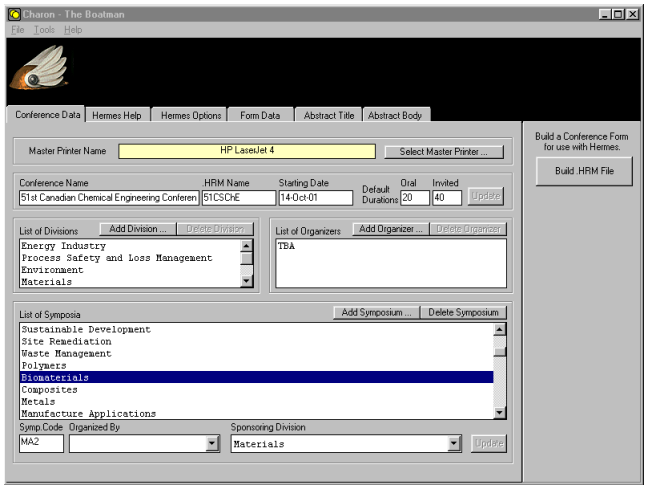


Figure 2.1 The Conference Data Screen within Charon

3. **Name of .HRM file** This will be used for distribution to authors and should be eight letters or less, *e.g.*,

```
51CSChE
```

4. **Conference Starting Date** This corresponds to the first day of the scientific program on which abstracts can be scheduled. Although it is displayed with only two year digits, the year must be **entered** using 4 digits, *e.g.*,

```
02-Jun-1997
10-Oct-2001

12-May-01 is WRONG
```

5. **Default Durations** These are for submitted oral and invited papers, *e.g.*,

```
oral            20        invited        40
```

Note that the length of any presentation can be overridden later within Charon or Tartarus (CSC Award lectures are 60 minutes), but it is convenient to specify early on the standard time slots to be used.

6. **List of Divisions** In recent CSC meetings this would correspond to:

```
Analytical Chemistry
Biological and Medicinal Chemistry
Chemical Education
Environmental Chemistry
Inorganic Chemistry
Macromolecular Chemistry
Organic Chemistry
Physical and Theoretical Chemistry
CIC/CSC Award Lecture
```

Note that, for CSC meetings, scheduling award lectures is best handled by creating a "virtual Division" called CIC/CSC.

For non-CSC meetings, the Division can be thought of as a major topic area, or field area.

Small conferences which really don't need a two tier classification scheme should still **create at least one Division**. The Division name should be the name of the Conference, *e.g.,* 34th SOUSCC.

7. **List of Organizers** Information on symposium organizers is important to authors (especially invited speakers), as they may know little about their invitation save that "Jane Doe" invited them. This information will also appear as a header for every symposium in the final program, so be careful of your spelling. At this stage names can be entered in any sequence, as long as the format is the same, *e.g.*,

```
Goddard, J,
Other, A.N.
Codding, P.W. and Patterson, J.
Patterson, J.
etc.
```

If the names of the organizers are not known ahead of time, you should still **create at least one organizer** called TBA or something similar.

8. **List of Symposia** When the `Add Symposium` key is pressed, the operator is prompted for the name of the Symposium. When the Symposium is selected from the list of Symposia, its code, the name(s) of its organizer(s), and the sponsoring Division can be specified.

The optional symposium code is a short, helpful mnemonic used in the generated program, abstract book, and web pages to reference a specific symposium. These codes should be **no more than 4 letters long** due to printing restrictions. In principle these codes can be any meaningful sequence. Optionally, despite the symposium code's true usefulness, this field can be left blank.

There is, for example, an accepted set of abbreviations for the different Divisions of the CSC. These can be found in any past conference program. Symposia codes within the Organic Division, for example, are generally OR followed by a one or two digit number. *e.g.*,

```
Organic Chemistry of Organometallics

OR3  Codding, P.W., Patterson, J.       Organic
```

There is a strong argument for avoiding the use of numbers in these codes. The order of appearance of symposia within the conference program may not always jibe with their assigned number. This results in the "appearance" of the symposia being out of order even though they are not.

Note: The General and Poster Sessions must be included as Symposia at this time. Each award lecture is also added here as a symposium under a "virtual" Division called, for example, Awards. They carry the internal code `Award`, but are not assigned an organizer. They are simply specified as being sponsored by the conference, *e.g.,* CSC. Hence:

```
Alcan Award Lecture

Award                              CIC/CSC
```

Remember to use the full citation for this award (e.g., `Merck Frosst Centre for Therapeutic Research Award`), as this is how it will appear in the final program.

Note: The scheduling of Award Lectures may require the later generation of some extra "virtual symposia". This issue is described in more detail in Chapter 4.

2.2.2 Hermes Help All the Hermes Help messages can be edited or modified to accommodate the needs of a particular conference. The default messages are those suitable for a CSC Conference and should not need adjustment. The `Submission Instruction` area is *extremely important*, and obviously unique to every conference. Very clear and specific details on the way in which an electronic abstract can be submitted (*e.g.*, web-upload, ftp) must be placed in this notepad. Deadlines for submission, addresses, web URLs and any telephone help lines can also be placed here. A suggested format is provided in Chapter 3. *Check this information very carefully.* Press `Update` when complete.

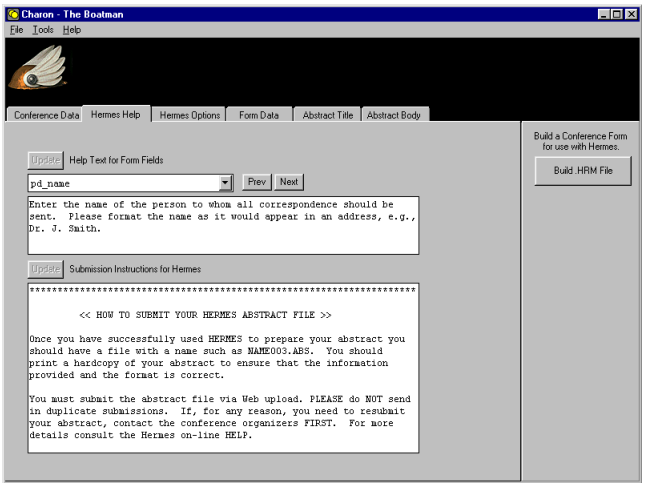


Figure 2.1 The Help Messages Folder within Charon.

2.2.3 Hermes Options The **Hermes Options** screen is designed to allow organizers of smaller mini-conferences or discussion groups to simplify or modify the information requested of submitting authors. Membership numbers may be unnecessary, or there may be no award lectures. The default settings are those typical of a CSC Conference. Click on the `Update` key when complete.

In version 2.6, support for new styles of abstracts has been added. This was done to support the needs of the CSChE conferences. Organizers can now choose the traditional

6 abstracts per page layout or the new 4, 2 or even 1 abstract per page. Further, new header formats (Title, authors and affiliations) are available. Also the font size of the abstract header and body can be selected. These selections must be made prior to distributing the .HRM file and must not be altered after that point.

CSC Header Style

A simulation study on the coupling between concentration polarisation and adsorption in tubular ultrafiltration membrane. **A. Beicha**, Curtin University of Technology, Riam road, 98000, Miri, Sarawak, Malaysia; **M.Z. Sulaiman** and **N.M. Sulaiman**, Chemical engineering Department, University Malaya, 50603, Kuala Lumpur, Malaysia.

CSChE Header Style 1

A simulation study on the coupling between concentration polarisation and adsorption in tubular ultrafiltration membrane.

A. Beicha, Curtin University of Technology, Riam road, 98000, Miri, Sarawak, Malaysia; M.Z. Sulaiman and N.M. Sulaiman, Chemical engineering Department, University Malaya, 50603, Kuala Lumpur, Malaysia.

CSChE Header Style 2

A simulation study on the coupling between concentration polarisation and adsorption in tubular ultrafiltration membrane.

A. Beicha[1], M.Z. Sulaiman[2], N.M. Sulaiman[2]

[1]Curtin University of Technology, Riam road, 98000, Miri, Sarawak, Malaysia.

[2]Chemical engineering Department, University Malaya, 50603, Kuala Lumpur, Malaysia.

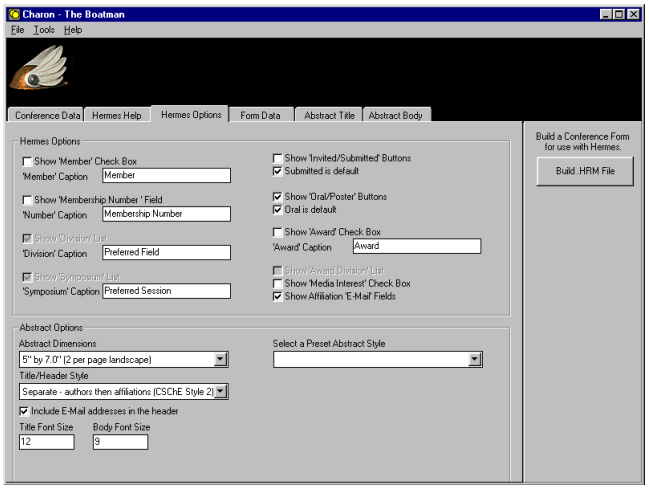


Figure 2.3 The Hermes Options Folder within Charon.

The field `Select a Preset Abstract Style`, sets the abstract options to the standard values for the type of conference selected.

2.2.4 Generation of the .HRM file Once the above database has been prepared, the corresponding .HRM file can be generated by pressing the `Build .HRM` File key. on the Conference Data screen. Changes to the .HRM file can be made at any time before distribution by pressing the key again. This procedure simply overwrites the existing file with the new version. If the organizer wishes to update the .HRM file (*e.g.*, add a new symposium) and distribute a new version, this can be done. Upon receipt of abstracts built using the old .HRM file, Charon will flag the abstract, and updates and modifications of the abstract can be made within Charon.

2.3 Distribution of the .HRM file The .HRM file is actually saved in two forms. Thus, for example, when the .HRM file is CSC80CAE.HRM is prepared, the corresponding file CSC80CAE.EXE file will also be generated. The latter is a self-extracting compressed version, and is much safer for distribution purposes, by e-mail, ftp or on diskette. Information on the distribution, installation and loading of the .HRM file is provided in Chapter 3. Note that, in the event that an author does not have access to the correct .HRM file, an abstract can be submitted using the SAMPLE.HRM file built into Hermes. Abstracts submitted using this latter format will be missing some information (*e.g.*, on Divisions, Symposia), but this data can be incorporated by the organizer at the receipt stage.

*Note: When O'Zone Software performs the initialization which is the normal case, the conference .HRM file will be bundled with the Hermes authoring software that abstract authors download from the O'Zone web site.

2.4 Abstract Receipt Abstract receipt is a stressful time. Hundreds of abstracts will be arriving during a very short period. About one third of all abstracts could arrive the last day All of these must be carefully handled so as to avoid loss. Duplicate submissions are a common feature of the electronic option, but this can usually be picked up later.

2.4.1 Hardcopy Abstracts If possible, hardcopy abstracts should be forbidden. The protocol for the handling of hardcopy abstracts is clearly at the discretion of the organizers. If they are accepted, we recommend assigning personnel to the task of transcribing hardcopy abstracts into an onsite version of Hermes rather than entering the data directly into Charon. The on-site use of Hermes allows Charon to be dedicated to the importation of already prepared electronic abstracts.

2.4.2 Non-Hermes Abstracts Despite all instructions, some authors will submit non-Hermes abstracts. These would typically be Word or Word Perfect files. What should be done with these abstracts is at the discretion of the organizers. Consider, however, that dealing with one non-Hermes abstract takes as long as importing 10 or 20 Hermes abstracts. Still, there are a few cases where it might be politically advantages to accept a few non-Hermes abstracts. Some authors who do not use Windows (for whatever reason) may complain bitterly. If possible, it is most efficient to assign the task of transcribing the non-Hermes abstracts into Hermes to the Symposium organizer.

2.4.3 Hermes Abstracts The development of a failsafe protocol for the importation of Hermes abstracts into Charon is critical to the success of the scheduling process. Whatever method is selected, it must provide a mechanism for protecting the original abstract, as received, so that in the event of a system failure, the database can always be repaired or even rebuilt. O'Zone Software will always maintain the original submitted abstracts on its web server as well as an off-site location. Still, the importance of regular and reliable backups cannot be overstressed.

2.4.4 Importing from ABS_NEW Upon installation of the Hermes Suite a directory `ABS_NEW` is created. All abstracts generated by Hermes and destined for importation into Charon should be moved into this directory. Charon can import new abstracts from any directory or disk, but as it does so *it removes the file from that location* and places it in `ABS_PROC` (name collisions are handled by changing the file extension). This feature was specifically introduced to avoid the otherwise distressing tendency of overworked organizers to import the same abstract several times. Thus, if `ABS_NEW` is empty, there are no more abstracts to import.

2.4.5 The Form Data Screen

Import Abstract To import an abstract from `ABS_NEW` into the database the operator presses the `Import Abstracts` button, which displays the default import directory

ABS_NEW. Abstracts can only be imported singly by design. This restriction was made to ensure that each and every abstract can be checked individually for format and content. A badly corrupted abstract file can be cleared from the screen (click on Clear) and reviewed or re-imported later. When an abstract is selected for import all the data provided by Hermes is drawn into the appropriate location on the Form Data screen. Charon contains a check routine that can pick up inconsistencies, omissions or missing information in an abstract, in which case the Damaged on Receipt flag will appear. Regardless, the operator can and should check the data on the Form Data screen, and also move to the Abstract Title and Abstract screens, to search for any problems. Minor problems of format or omission can be fixed on the fly, and the *Damaged on Receipt* flag switched OFF. More serious problems can be left to a later time, in which case leave the flag switched ON.
The Division, Symposium areas (bottom left) contain the choices provided by the submitter. The organizer can override these choices, if necessary, while still retaining a record of the original selection. Oral/poster choices can also be reassigned, and the duration of a talk can be set to any special value if desired. Student Awards are confirmed in a similar way.

Author names and addresses sometimes need editing. The format should be consistent, *i.e.*, family name followed by initials (Jones, P.A.). There should be a link from every name to at least one address (often single authors fail to make this link). More and more error checking is being placed into Hermes the authoring application but invariably authors are creative.

By moving to the **Title** and **Abstract** screens the operator can check for format as well as other problems. Many authors break into CAPS for Titles. Two functions on the Tool menu can be used to convert the Title letter case. In each case, the converted title is placed after the original title. This allows the original title to be used as a reference to ensure that the conversion is correct. The original title should then be blocked and deleted.
In the abstract some editorial work may be necessary. For example, some authors fail to leave a space between the address section and the abstract (such is their desire to fill the space). The decision on style *vs.* substance is in the hands of the organizer. If there appears to be a missing or truncated abstract (a bad graphic), the organizer should, as noted earlier, leave the Damaged on Receipt flag ON, but can still continue to process the abstract into the database. The operator always has the choice of saving an abstract into the database of clearing it completely from the screen (and the database). Any abstract can always be overwritten later (see Delete Current and Change ID).

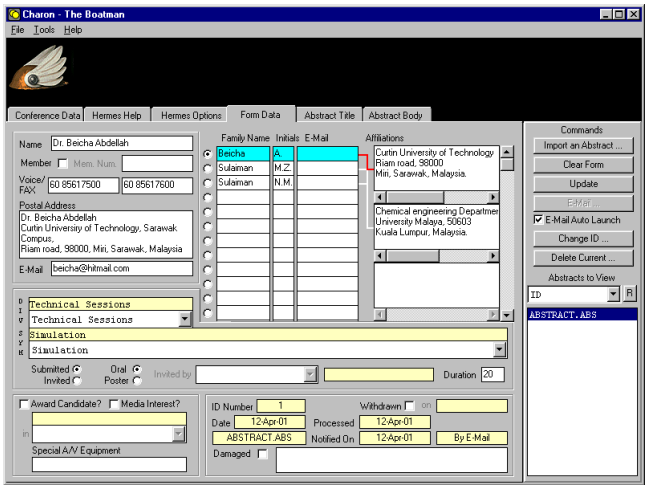


Figure 2.4 The Form Data Folder within Charon, showing sample input.

Process and Save Once the decision has been made to proceed with saving the abstract into the database, the operator presses the **`Process and Save`** key. This invokes several functions.

1. The full Hermes abstract is *moved* from the `ABS_NEW` directory to the `ABS_PROC` directory. At the end of the day (and the conference!), all abstracts should have been moved from `ABS_NEW` to `ABS_PROC`.

2. All the data contained in the Hermes abstract file is distributed to the appropriate locations in the database (in the `DATABASE` directory). The abstract is also assigned a permanent ID number (not to be confused with the abstract sequence number in the abstract book and schedule - that comes later).

Notification of Receipt Not necessarily, but usually, at this time a notification of receipt can be shipped out. Any abstract with a valid e-mail will display an `E-Mail` option. If the `E-Mail Auto Launch` check box is marked, the E-Mail dialog will open as soon as you `Process and Save` an abstract. Otherwise the dialog can be invoked by clicking the `E-Mail` button.

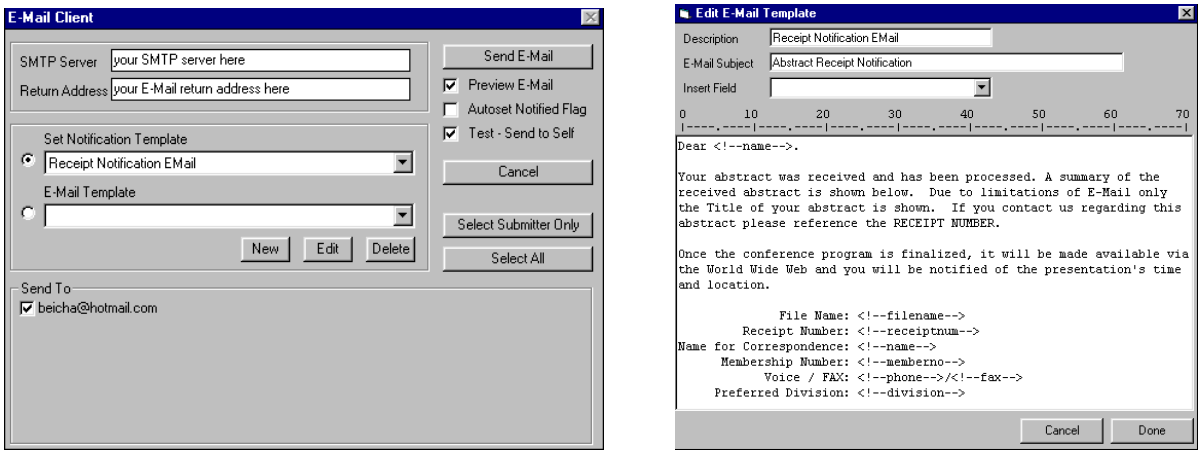


Figure 2.5 The E-Mail Dialog within Charon (left) and the E-Mail Template editor (right).

The E-Mail system uses templates that can be populated with information taken from the conference database. A standard Receipt Notification E-Mail template already exists, although you might choose to alter it. New templates can be created via `New`, and existing templates can be edited by selecting them in the `E-Mail Template` drop down list and clicking `Edit`.

When creating a template, type only the generic text. Any items that are specific to the person receiving the e-mail should ideally use Inserted Field data. This way, you can build up a library of common e-mail templates.

The Conference Diary This version of Charon requires that abstracts be loaded *one at a time*. For newcomers to the software this is a slightly slower but safer procedure. It is also both prudent and useful, though optional, to keep a hardcopy (hand-written) summary - a Conference Diary - in which the following information is noted:

ID number
Name of Correspondent
Abstract Filename
Date of processing
e-mail address of correspondent
Any serious difficulties (corrupted graphics, truncated in transmission)

At the end of the conference, this diary will provide a lasting and sometimes amusing record of the entire abstract receipt process. *The tally of abstracts in the logbook should always match that in the database.*

Delete Current and Change ID At any time an abstract in the database can be removed and replaced by a new (amended or repaired) version. A discovered duplicate

abstract can also be removed and replaced by a completely new abstract. In this way, it is possible to ensure that the total number of abstracts in the database is equal to the last ID number in the database (and the Conference Diary). The deletion/change ID procedure begins by clicking on the `Delete Current` key. This will delete all the data corresponding to a particular ID. (Note that once an ID is generated, it is never removed from the database.) A new (or replacement) abstract can then be imported into Charon, and the `Change ID` key can be used to alter its ID to any new value. *Care should be exercised in these manipulations!* In the event that the `Change ID` option is invoked on the last (*i.e.*, most recent) abstract in the database, this original ID number will remain available for future use. Thus, for example, if there are 802 IDs in use, and you wish to replace abstract ID 412 with a new entry:

1. `Delete Current` abstract with ID 412.
2. `Import` a new abstract (with ID 803).
3. `Change ID` of newly imported abstract from 803 to 412.

After this sequence, ID 803 will still be available for an incoming (new) abstract.

Abstracts to View The Abstracts to View Bar on the bottom right of the Form Data screen provides a list with options similar to:

```
All Processed
By ID
By ID Range
Last 10 ID's
Last N ID's
By Date
By Date Range
By Correspondent
By Authors
By FileName
By Division ID
By Division Name
By invited/division
UnNotified
Award Candidates
Media Interest
A/V Equipment
Unassigned
By invited
Membership
By Award/Division Name
By A/V Equipment/Division Name
Contain Graphics
Damaged on Receipt
```

These options allow the operator to assess the status and content of the abstracts by major groups. By clicking on any one of these group options, all abstracts in that category are shown in the menu below. Clicking on the `Print List of Abstracts` button on the main `File` tile (top left of main menu bar) opens a menu box which allows the operator to print, as hardcopy or as an RTF file, a listing of any set of papers within a particular category. Options for what information is to be provided are user-selected.

Database Statistics By clicking on the Tools key (top left) one can access (and print) a full statistical review of the contents of the conference database. This information is vital, and routine and regular checks of the entire system should be made throughout the abstract receipt/scheduling process.

Chapter 3 - Hermes

3.1 Distribution Typically once the call for papers has been announced, O'Zone Software will prepare a set of pages for the conference on their web site. These pages, located at `http://www.ozonesoftware.com`, will allow authors to

1) download `HSETUP.EXE`, the Hermes authoring software plus the conference specific .HRM file. Authors will install Hermes on their Windows computer by running `HSETUP.EXE`.

2) submit their completed abstracts via web-upload. Web upload is the preferred submission method because it is easy for authors, very reliable, allows the collection of redundant contact information, and allows the authors to be given meaningful error messages in the event that something does go wrong.

Conference organizers should link from their conference web site to `www.ozonesoftware.com`. On this site there will be a links to various conferences. Authors should be instructed to follow the link for the conference to which they wish to submit an abstract.

3.2 Installation of Hermes

The name of the file authors retrieve is `HSETUP.EXE`. This is a self-extracting file. Suggested installation instructions for the user are:

1. From Windows Explorer locate the downloaded copy of `HSETUP.EXE` and double click on it. This will extract all the contained files to a temporary directory (which will be deleted on completion) and, by default, will install the Hermes program plus templates to c:\hermes.

2. Authors can run Hermes by clicking in sequence, Start, Program Files, Hermes, Hermes 2.x.

WIN 32S Extensions WIN 32S extensions are available from the HERMES World Wide Web site. These are only necessary for computers using Windows 3.1.

Past experience has led us to conclude that the success rate for (unassisted) installation by users is >95%. Most problems encountered thus far seem to have stemmed from users failing to close all other applications before running setup.exe. A warning to this effect has now been included in the setup procedure. Also a more intelligent version of setup.exe has recently (2001) been substituted that avoids many of these problems. A very few configurations have remained totally resistant to installation. For these cases we recommend that authors try another computer.

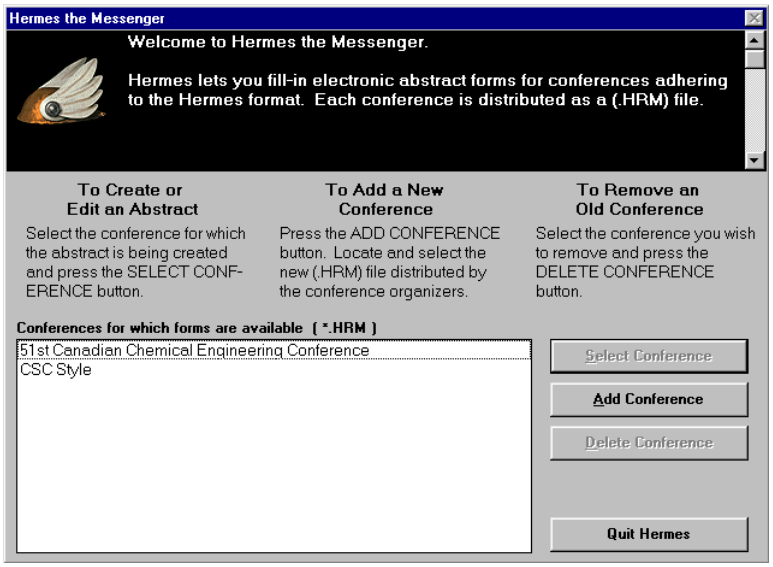


Figure 3.1 Opening screen of Hermes V2.6, showing selection of Conference forms.

3.3 Operation of Hermes There is no User Manual for Hermes. There is, however, extensive on-line HELP built into the program, and every effort has been made to make the program as simple as possible to use. Nevertheless the organizers should be prepared to make themselves available, either by phone or e-mail, during the critical abstract submission period to assist any author who is experiencing difficulties. Based on the kind of problems/curiosities present in the abstracts submitted using Hermes V1 we have tried further to simplify and clarify the new version. To this end the `.HRM` file generated by Charon contains a variety of messages which the organizers may wish to expand or replace. Critical, of course, is the information on submission - "how, when and where". This must be prepared carefully so as to avoid any misinterpretation.

A new feature of Hermes V2 is the opening screen, which allows the user to select the conference for which abstracts are to be generated. If the .HRM file for your conference has been loaded correctly, the user can click on the desired form and continue.
The main screen of Hermes consists of a series of folders.

1. Correspondence Data
2. Symposia
3. Authors/Addresses
4. Title
5. Abstract
6. Submission

These areas correspond to what one would find on any conventional hardcopy abstract. Upon opening any one of these folders the user is prompted for specific information.

Folder 1 (Correspondence) This data should be simple, but many authors wonder about the significance of the name "at the top". This name is for correspondence only, and will never appear in the conference program. A secretary or friend of the author will do fine. It is to this person, and to this address, that all correspondence will normally be sent.

Figure 3.2 The Correspondence Folder within Hermes, showing sample data.

Folder 2 (Symposium Data) This screen allows users to select the Division and Symposium under which they prefer their abstract to appear. Presentation formats, oral versus poster, media interest, audio/visual needs can also be specified.

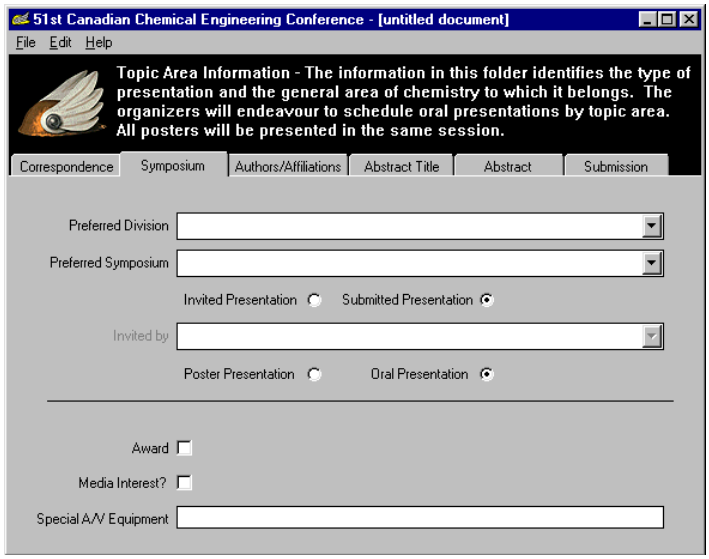


Figure 3.3 The Symposium Folder within Hermes, showing typical CSC data.

Folder 3 (Authors/Affiliations) This screen has caused some minor interpretational problems, nearly all of which are easily repaired upon receipt by Charon. In Hermes V2.6 additional error checking has been added to catch many of the common mistakes.

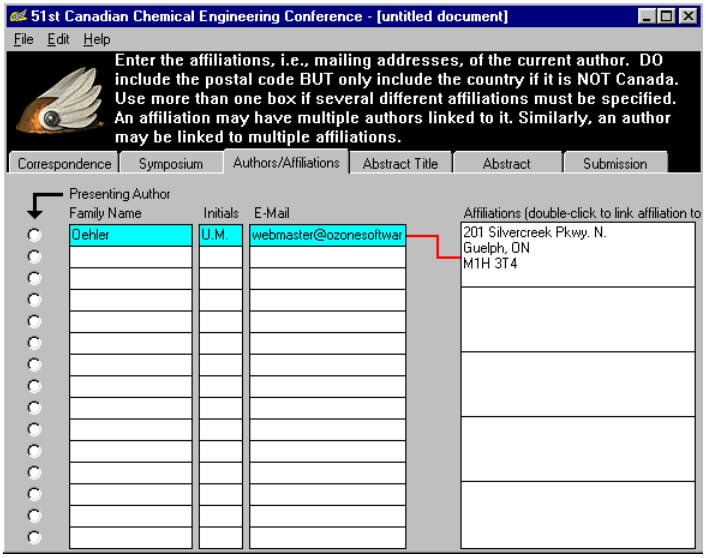


Figure 3.4 The Author/Affiliations Folder within Hermes, showing sample input.

Folder 4 (Title) This should be easy enough, although authors seem to take delight in using CAPs, which is perhaps a throw-back to the old days. Error checks warn authors when titles appear to be all caps. Additionally, commands in Charon make converting to mixed case fairly easy.

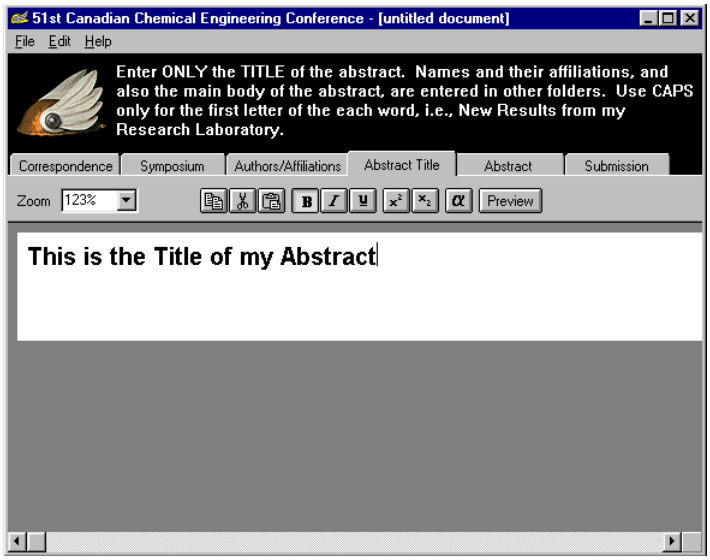


Figure 3.5 The Title Folder within Hermes, showing sample input.

Folder 5 (Abstract) Authors are prompted to fill out the `Authors/Affiliations` and `Title` screens first as information on these screens reduces the space available for the abstract. This prompt disappears when they have complied. All normal editing features (**bold**, $_{subs}$, ^{supers}, *italics*, cut and paste) are available for preparing the abstract, as well as zoom and preview. There is, however, *no* font control, and users who write the abstract in another word processor and cut and paste it into Hermes will lose their font and formatting selections. This approach is vital to the WYSIWYG concept. If the abstract fits the screen, it is acceptable, and will appear exactly as written in the abstract book. Abstracts received at CSC95 and CSC96, prepared by conventional word processors, were subject to every conceivable manipulation of font and font size (not to mention abstract length). These all required careful editing to ensure that they were within the space limitations of the final abstract book. A single graphic can be incorporated, *via* cut and paste, from any Windows drawing or modeling software (*e.g.*, ChemWindows, ChemDraw, Corel Draw, Presentations).

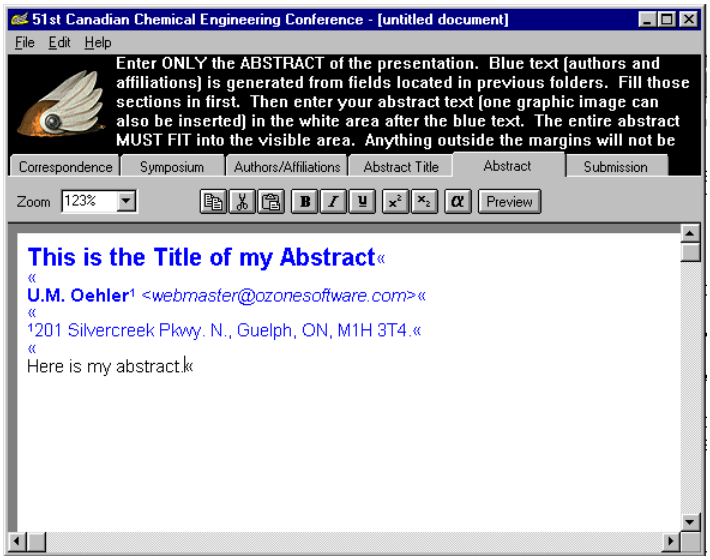


Figure 3.5 Abstract Folder within Hermes, with sample abstract in draft mode.

Folder 6 (Submission) This information is prepared by the organizer from within Charon, and is introduced to Hermes *via* the .HRM file. Shown below is the kind of information that should be present in this section.

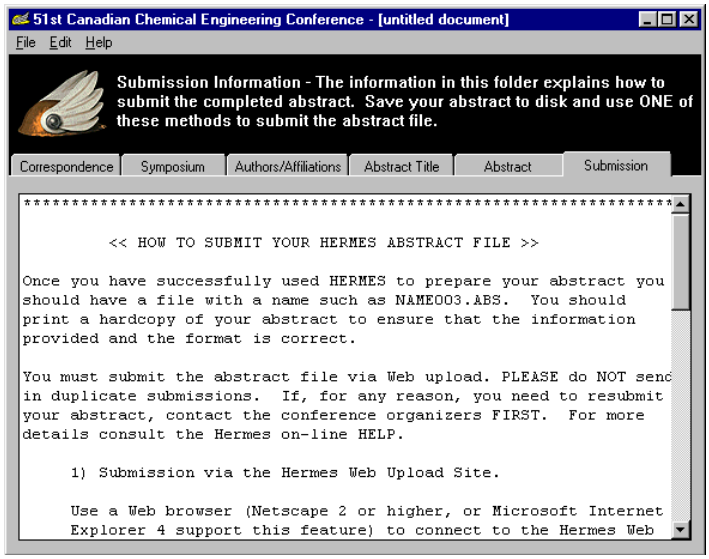


Figure 3.6 The Submission Details Folder within Hermes, showing sample information.

3.4 Electronic vs. Hardcopy For conference organizers the strength of the Hermes Suite lies not so much in the electronic abstract itself as in the way in which the abstract couples with the processing and scheduling software Charon and Tartarus. Abstracts prepared via Hermes require, in most cases, no editing by conference organizers. They

import smoothly into the system and organizers can concentrate on scheduling issues. Once the scheduling is done, hardcopy and web pages flow out of the system with no further user intervention required.

The use of an electronic abstract system such as the Hermes Suite can save conference organizers a great deal of time and effort. By no means will all of the contributors to a conference agree with the approach. Others may like the idea but not the reality of Hermes, either because the software does not run on a MAC or because it is perceived to be too difficult or too inconvenient to download and/or operate. Perhaps, within a short time, more flexible and interactive software will be available for use on the World Wide Web, thereby offsetting the need for a PC based program.

Non-Hermes abstracts should not be widely encouraged as some transcription will be necessary. Nonetheless, the whole idea behind Hermes is to provide authors with a choice. At the present time, it appears that most delegates to a CSC Conference will use Hermes, if encouraged, to prepare and submit an electronic submission. It is important for organizers to remember the sensibilities - and the rights - of those who elect not to use Hermes. Allowing abstracts to be submitted in other formats by these select few should be considered.

Chapter 4 - Tartarus

4.1 Introduction As the name Tartarus suggests, the scheduling of a conference, along with the preparation of the program and abstract book, makes Hades seem like an attractive location for a post-conference vacation. The purpose of the Tartarus program is to make this scheduling and publishing process as simple and stress-free as possible. Tartarus was designed with the format of a standard CSC Conference in mind, and while variations are possible, this version of the Hermes Suite remains restricted to meet specifically the objectives of such a Conference. Tartarus provides the following output:

Hardcopy Material

Complete Conference Program, standard CSC (3-column) format
Full author index, standard CSC format
All signs for meeting rooms on a per half-day basis
Full Abstract Book, standard CSC (6,4,2 or 1 abstract(s) per page) format

World Wide Web Material

Full Conference Program, organized by different criteria like author, day and Division, as HTML files
Full Abstract Book (abstracts embedded as GIF images in HTML files)
CD version of abstract book available at cost through O'Zone Software

However, the power of Tartarus lies not so much in its formatted output, as in the fast, simple and highly interactive way it allows the scheduling of presentations to be carried out.

4.2 Operation Upon loading Tartarus, by double clicking on the appropriate Windows 95 icon, a series of folders appears on the screen.

```
1.   Order of Divisions
2.   Order of Symposia
3.   Symposium Schedule
4.   Print Reports
```

4.2.1 Order of Divisions Tartarus opens to the Order of Divisions folder, and displays a list of tiles, each one of which represents a societal Division. These can be reordered in desired manner by dragging the tiles with the mouse. The typical ordering of Divisions in the Program of a CSC Conference is:

```
CIC/CSC Award
Analytical Chemistry
```

```
Biological and Medicinal Chemistry
Chemical Education
Environmental Chemistry
Inorganic Chemistry
Macromolecular Chemistry
Organic Chemistry
Physical and Theoretical Chemistry
```

Essentially the Divisions are typically listed alphabetically, with all CIC/CSC award lectures leading the way. This latter feature is critical, so that the exclusivity of these presentations can be properly handled. Clicking on `Save Current Order` does just that.

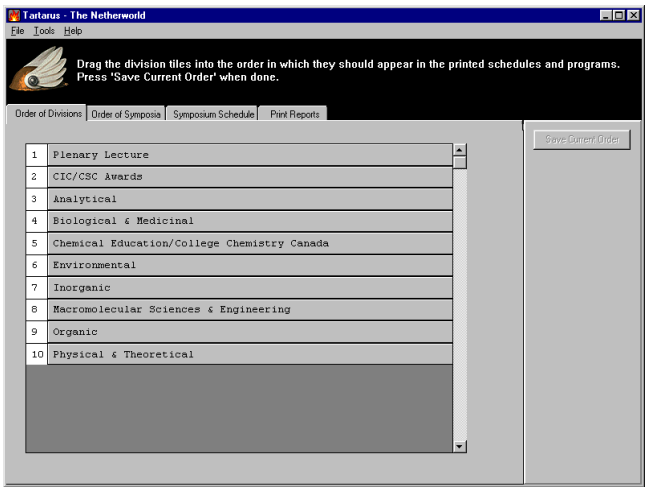


Figure 4.1 The Order of Divisions Folder within Tartarus, showing a sample listing.

4.2.2 Order of Symposia A white text box appears at the top of the screen when this window is opened. If the operator clicks on this box and scrolls down the list of Divisions he/she can select any one of the societal Divisions. Clicking on any Division produces a slate of tiles corresponding to the symposia within that Division. As with the Divisions the order of the symposia in the program can be adjusted simply by moving the tiles with the mouse. The order of symposia, which can be modified at any time up to the final printing, can be saved by clicking on the `Save Current Order` key. If the preliminary construction of the .HRM file was done judiciously, there should be no need for any adjustment at this time. Note that the codes for Symposia are built into the .HRM file at the early stages of conference planning. Organizers are urged to decide early on these codes, and be prepared to live with them.

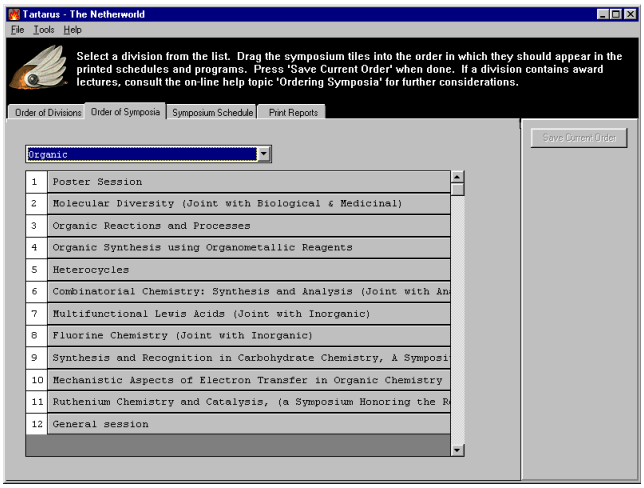


Figure 4.2 The Order of Symposia Folder within Tartarus, showing a sample listing.

Note: For CSC Conferences, General Sessions and Posters (in that order) are placed at the end of the list of symposia. Outside of that convention, the ordering of symposia in the program is at the discretion of the organizers. Bear in mind that this order simply establishes the sequence of printing for a given half-day session in the event that all symposia are running. For example, if only two symposia are running on the last afternoon of the conference, their ordering will be as established here.

Note: CSC Award Lectures do not appear in this sequence. Those lectures which preempt all others can be slated within the CIC/CSC Award "Division". Others, such as the Alcan Award, only preempt other lectures within the Inorganic Division. Such singularities are best handled in an *ad hoc* manner (see section 4.2.4).

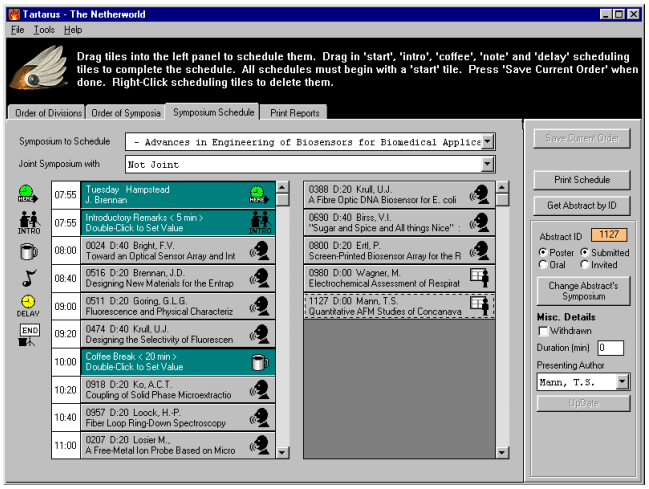


Figure 4.3 The Symposium Schedule Folder with Tartarus, illustrating a partially scheduled symposium.

4.2.3 Symposium Schedule This folder, which is the most detailed and important within Tartarus, opens to a white text box; scrolling down affords a list of all the symposia in the Conference. The organizer can chose any one of these symposia and, by clicking on his/her selection, can open the current contents of the symposium, *i.e.*, the papers submitted and invited to that symposium. The screen consists of three panels. There are two panels for the presentations, one for scheduled and one for unscheduled. The third panel on the right contains a series of control keys.

4.2.3.1 Sorting Papers into Symposia The ordering of papers is developed, as above, by using the mouse to move tiles, each tile corresponding to a paper or poster (note the symbolic icons representing oral *vs.* poster presentations). In essence the act of moving a tile from the right to left panel builds the sequence of presentations. It is entirely possible, if not probable, that the list of papers in the symposium is incomplete or incorrect because:

- Invited speakers have failed to submit an abstract
- Authors have inappropriately submitted their paper to the current symposium
- Authors have inappropriately submitted their paper to a different symposium

The first problem is beyond the control of software; the organizers must be alert for delinquent speakers and track them down. The second problem can be rectified by clicking on the tile corresponding to a misplaced paper and then clicking the `Set Abstract Symposium` key. This opens a small screen and scroll bar, which may be used to reassign the paper to the correct symposium. The third problem can be fixed by using the `Get Abstract by ID` key. Clicking on this key opens a prompt for the ID number of the paper which should be relocated to the currently active symposium.

4.2.3.2 Building a Session The construction of a symposium begins with a slate of unscheduled papers, which can be updated as late arrivals show up. Shifting and shuffling the tiles on the left panel creates the order of presentation. The following control icons on the extreme left of the screen effect the following operations:

Session Start Moving this tile into the left panel, and double-clicking on it opens a control box into which the operator types the following data:

```
Session Chairperson(s):
Starting time:
Duration if poster session:
Starting Day:
Room:
```

Note: The Starting Day for the Conference (as opposed to the symposium) is defined within Charon (Conference Data screen). Also times are entered using a 24 hour clock.

Right-clicking on the tile will remove it.

Introductory Remarks This icon provides a slot for the symposium organizer to open the first session with a *few* well-chosen words. The duration can be modified from the default value of 5 min by double-clicking the tile. Right-clicking on the tile will remove it.

Coffee Break This is a generic coffee or nutrition break, the duration of which can be modified from the default value of 20 min by double-clicking the tile. Right-clicking on the tile will remove it.

Note This icon allows organizers to insert a special comment plus, if desired, a time slot for some special event, *e.g.*, a vote of thanks, a small presentation, *etc*. A few words can be inserted directly into the program to announce this event. Optionally, one can also have the time displayed as for abstracts and a header, as appears for Symposia, can be turned on.

Delay A delay is inserted when the organizers wish to incorporate a pause in the program, perhaps because of a plenary lecture elsewhere. Nothing will

appear in the final program, but the start time of the next paper will be altered accordingly.

End of Session This adds a note saying "End of Session". When placed at the end of a session, it allows readers to determine the duration of the last presentation.

When an abstract tile in the unscheduled column is highlighted, certain information can be edited.

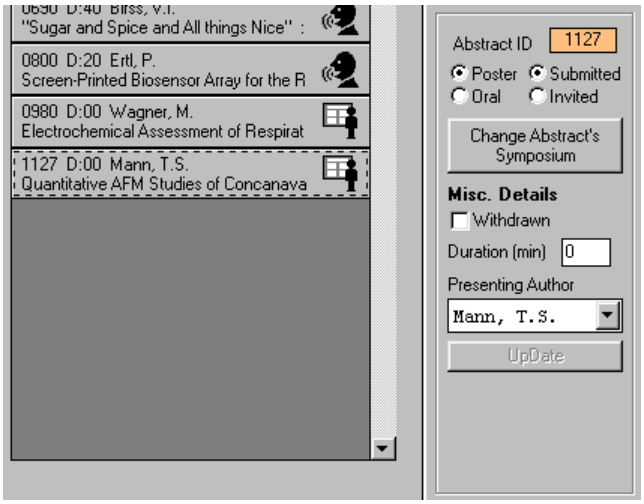


Figure 4.4 Editable information for unscheduled abstracts.

4.2.3.3 Presenting Author Clicking on the `Presenting Author` key opens a scroll box which allows the organizer to change the name of the presenting author from that indicated in the abstract. Clicking on the `Update` key updates the relevant tile. Oral *vs*. poster icons will also be refreshed at this time.

4.2.3.4 Withdrawn Clicking on `Withdrawn` retains the position of a paper in the symposium, but it is flagged as being withdrawn both in the Final Program and the Abstract Book. This is useful late in the scheduling process once the schedule has been made public. When the schedule is published, each abstract is assigned a sequence number based on its order of appearance. Readers associate the sequence number with a specific abstract. Removing even one abstract will throw off the sequence numbers of all the abstracts that follow the it. Therefore, once the schedule is public, it's better to "withdraw" abstracts.

If the schedule has not yet been made public then the paper can be eliminated entirely from the database by deleting it.

4.2.3.5 Save Current Order Clicking on the `Save Current Order` key at any time during a scheduling session saves the current schedule to disk. Remember to make regular back-ups.

4.2.3.6 Print Schedule Clicking on the `Print Schedule` key opens a control box with three print options.

1. A printout of the symposium program, as it will appear in the final program. In this format, there is no delineation between sessions, and delays are specifically highlighted. Papers are identified by their ID rather their final sequence in the program. This printout is mainly designed to allow the organizer an opportunity to review format.

2. A text printout of current status of the symposium, broken down by sessions. This format is convenient for hardcopy transmission to symposium organizers.

3. An ASCII file containing the current status of the symposium, broken down by sessions. This file is also convenient for e-mail or ftp transmission to symposium organizers.

4.2.4 Award Lectures The scheduling of Award Lectures can be handled in one of three ways.

1. As described in Chapter 2, we recommend that all Award lectures initially be assigned to a "virtual" Division named CIC/CSC. Award winners may not specify this Division in their abstracts (they tend not to notice such details!), but the Division should exist, so that the organizers can assign to that Division any lecture they wish. Typically, those awards presented on the Sunday of a CSC Conference (first day), and which are not part of any symposium, can be allocated to this "Division". The "Symposium" CIC/CSC Award lecture can then be scheduled like any other, with suitable annotations (Notes).

2. For Award lectures that run at the same time as other symposia, but that are meant to be exclusive across a Division, we recommend the generation, by using Charon, of a new (uncoded) symposium, *e.g.*, the Alcan Lecture. This generation need not be done until well into the scheduling period (February/March for a CSC meeting), indeed early on in the development of the conference it may not be known which Award lectures are to be handled in this way. Once generated, this new symposium can be located (see

section 4.2.2) at the top of the list of symposia in that Division, so that its scheduling takes precedence over all other sessions. It is then up to the organizer to ensure that all other sessions in that Division start after the Award lecture has finished.

3. For Award lectures where there is no special exclusivity, the paper can be assigned to any symposium which the organizer feels is appropriate (on the basis of content). Suitable Notes can be used to introduce this presentation.

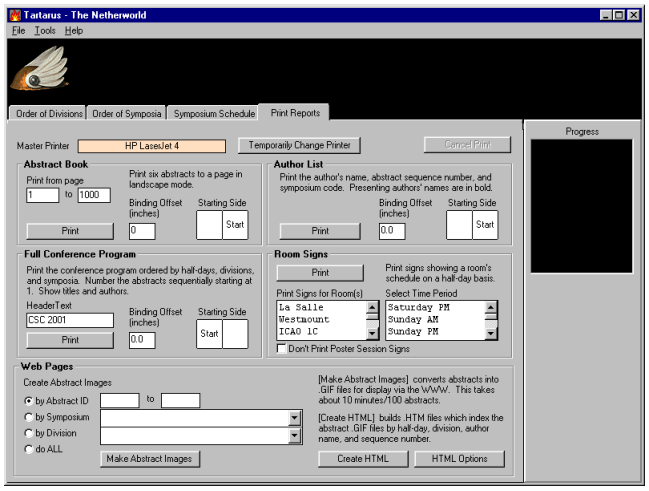


Figure 4.5 The Print Reports Folder in Tartarus.

4.3 Print Reports Once all previous stages in the scheduling have been completed, the publishing of the program, in hardcopy and electronic format, becomes a relatively routine matter. Opening the Print Report Folder reveals a screen with the following options:

Print Conference Program This option builds and prints the full conference program, from start to finish. Partial printouts are *not* possible, as the program would have to be built every time in any case. This print process requires 2/3 min per page depending on the speed of the computer. In the final program papers are now numbered according to their sequence in the program rather than their ID. If this print operation is invoked with only a partially scheduled program, only those papers that are scheduled will appear. This nonetheless may be a useful exercise in order to ensure that the desired sequencing is being achieved.

Print Author List This option prints the full author index for the program, at whatever stage the scheduling has reached.

Print Abstract Book This option prints the abstract book. Here there is control over which pages of the abstract book are printed. Remember that abstracts are numbered according to their sequence in the program, not their ID.

Print Room Signs This option prints all the rooms signs for any and all of the rooms assigned to the Conference. This printout is by room, on a per half-day basis. You can highlight the rooms and periods for which signs should be printed.

Web Pages Web pages consist of both HTML pages and GIF files. The GIF files are used to display a WYSIWYG view of the submitted abstracts. This section allows the organizer to generate web pages searchable by several criteria. The abstract GIF files can be generated by one of several ways:

1. By ID Range
2. By Symposium
3. By Division
4. Do All

Initially, option 4 can be invoked. This is a slow process, as it requires that a GIF file be generated for each and every abstract. Later on repairs or additions of groups of abstracts or specific abstracts can be made by selecting one of options 1, 2 or 3. Yet again, option 4 can always be invoked. Once the option has been invoked, clicking on the `Make Abstract Images` key starts the replication process. When this is complete, clicking on the `Create HTML` key builds all the necessary HTML files for the entire Web version of the program.

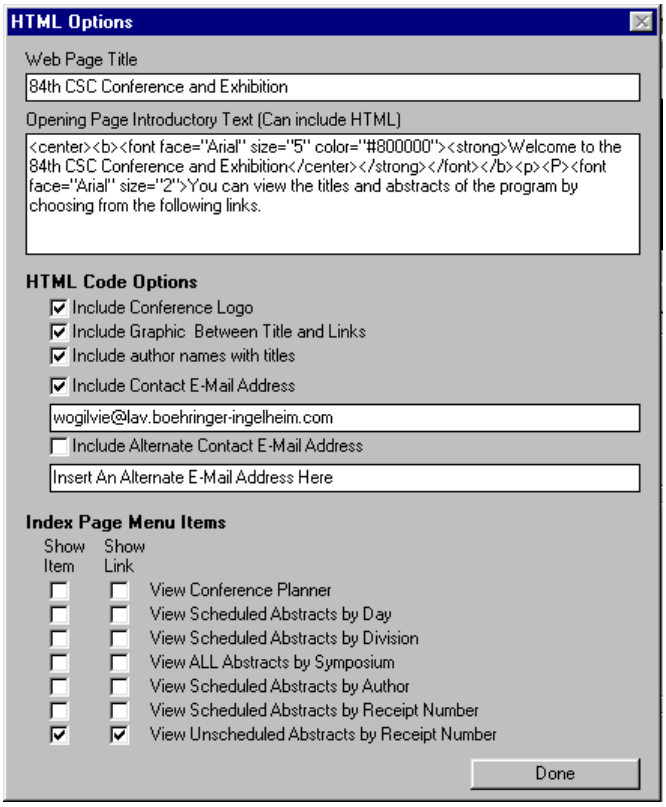


Figure 4.6 HTML Generation Options

The generated HTML creates the following views of the schedule as determined by the selected options under the HTML options dialog.

1. Conference Planner (half-days horizontally, symposia vertically, with links to the schedule at the intersections.
2. Abstracts by Half-Day (Monday AM, Monday PM, Tuesday AM, etc.)
3. Abstracts by Division
4. ALL Abstracts by Symposium (Designed for viewing by symposium organizers. The view shows abstracts numbered with their receipt numbers and includes both scheduled and unscheduled abstracts).
5. Abstracts by Author
6. ALL Scheduled Abstracts by Receipt Number (Designed for viewing by symposium organizers).
7. ALL Unscheduled Abstracts by Receipt Number (Designed for viewing by symposium organizers).

Temporarily Change Printer Early on in the program planning process the choice of the Master printer is made. This determines the reference set of font metrics that will be

used throughout in order to control the appearance and pagination of the abstracts and schedule. Using this option allows the organizer to print the various reports on any printer but using the font metrics of the Master Printer. For most 600dpi or better printers the text will look fine. On some printers which differ markedly from the Master Printer, letter spacing may appear a bit off. Some letters may seem too close together while others will appear too far apart. This can occur because the widths of corresponding letters on the two printers differ significantly. If the final prints are done on the Master Printer or to a PDF file, these oddities will not occur.

Database Statistics By clicking on the Tools key (top left) one can access (and print) a full statistical review of the contents of the conference database. This information is vital, and routine and regular checks of the entire system should be made throughout the abstract receipt/scheduling process.

HTML Files Examples of the HTML files generated for distribution on the World Wide Web are shown below. Note that there are four .GIF files located in a subdirectory off the HTML directory.

1. BACK.GIF
2. LOGO.GIF
3. BULLET.GIF
4. BAR.GIF

These files can be interchanged (with retention of the names indicated) by any other GIF files the organizers wish to use. Those provided here represent system defaults.

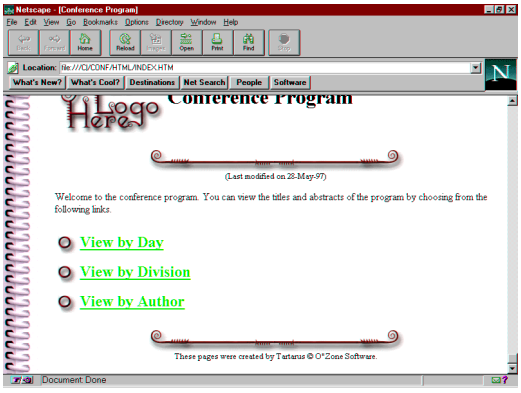


Figure 4.5 Sample index page (default .GIF files) for World Wide Web Version of program, as viewed within Netscape 3.0.

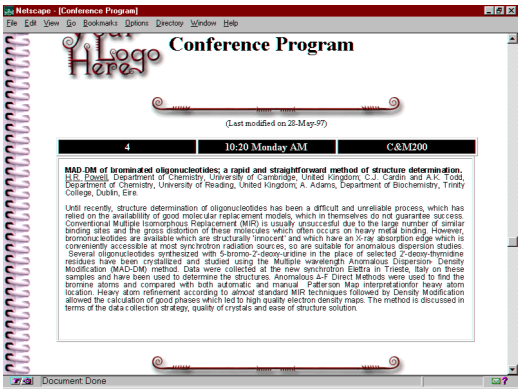


Figure 4.6 Sample abstract page (default .GIF files) for World Wide Web Version of a conference program, as viewed within Netscape 3.0.

Appendix - Sample Printouts

Attached are samples of the formatted output from the Hermes Suite, using a partial database provided by the organizers of a CSC Conference. No attempt has been made to edit the abstracts for consistency, style or typographical errors. Note that the fonts and styles correspond specifically to those used by the Canadian Society for Chemistry. Other organizers may wish to pursue alternative formats, in which case they should contact O'Zone Software.

Sample 1 Full Conference Program (single page, 3 columns).

Sample 2 Author list (single page, 3 columns).

Sample 3 Abstract Book (single page, landscape, 6 per page).

Sample 4 Room Sign (single session, 2 pages).

Sample 5 Database Statistics (2 pages).

Saturday PM

Plenary Lecture

ICAO 1A

Plenary Lecture

Chair - Y. Tsantrizos

20:00 Opening of Conference - R. Andersson

20:05 Opening Remarks - Y. Tsantrizos

20:10 Public Acknowledgement of Award Winners - T. Chivers

20:15 Introduction of C. Walsh - M. Bös

20:20 0001 *Nonribosomal Peptide Antibiotics: Enzymatic Strategies for Assembly* **Walsh CT.**

21:15 End of Session

21:15 Opening Mixer

Sunday AM

CIC/CSC Awards

Outremont

CIC Medal

Chair - V. Smith

Introduced by V. Smith

11:20 0002 *Race for the Photonic Chip* **Ozin GA.**

12:00 End of Session

Analytical

AN1 Hampstead

Spectroscopy and Imaging of Surfaces (Including Electrodes)

Organizer - D. Bélanger & B. Lennox
Chair - B. Lennox

08:55 Introductory Remarks

09:00 0003 *SPECTROSCOPIC AND ELECTROCHEMICAL STUDIES OF MONOLAYERS AND BILAYERS OF AMPHIPHILIC SURFACTANTS AT A GOLD ELECTRODE SURFACE* Zamlynny V., Burgess I., Li H.-Q., Horswell S., Lachenwitzer A., Szymanski G., **Lipkowski J.**, Majewski J., Satija S., Ivkov R.

09:40 0004 *Probing Electronic Properties of Adsorbed Molecules with Surface Plasmon Resonance Spectroscopy* Wang S., Boussaad S., Wong S., **Tao N.J.**

10:20 Coffee Break

10:40 0005 *In-situ Investigation of Adsorption Properties of Block Copolymer Amphiphiles by Surface Plasmon Spectroscopy (SPS)* **Advincula R.**, Park M., Knoll W.

11:00 0006 *Second harmonic generation spectroscopy of chemically modified Si(111) surfaces* **Mitchell S.A.**, Mehendale M., Villeneuve D.M., Boukherroub R., Flueraru C.P.

11:20 End of Session

AN4 Lachine

Higher Throughput Analytical Techniques

Organizer - J. Visentini
Chair - J. Visentini

Microchip Technologies

08:35 Introductory Remarks

08:40 0007 *Increasing LC/MS Sample Analysis Throughput: From Columns to Microchips* **Kapron J.T.**

09:20 0008 *A novel approach to DNA Transfection of E.Coli DH5α cells using a microchip.* **Majid E.**, Attiya S., Harrison D.J.

09:40 0009 *Working Towards a Simple Immunoassay on a Micro Fluidic Chip* **Roos K.P.**, Skinner C.D.

10:00 Coffee Break

10:20 0010 *Microfabricated Electrophoretic Devices for Rapid DNA and Protein Analysis of Molecular Diagnostic Importance* **Landers J.P.**

11:00 End of Session

AN7 Cote St. Luc

NEWs in Analytical Chemistry

Organizer - C. Lucy
Chair - C. Lucy

08:35 Introductory Remarks

08:40 0011 *Expanding the Utility of Sol-Gel Entrapped Proteins for Bioanalytical Applications.* Flora K.K., Bendiak G.N., Keeling-Tucker T., **Brennan J.D.**

09:00 0012 *Surface Interactions at Ultrathin Organic Film Interfaces* **Badia A.**

09:20 0013 *Comprehensive Multidimensional Gas Chromatography* **Górecki T.**, Harynuk J.

09:40 0014 *Analysis of Cytochrome P450's using LC-MS and MALDI-TOF: Tools for the Identification of Covalent Adducts* **Bateman K.P.**, Wilke M., Chauret N., Ouellet M., Percival M.D.

10:00 0015 *New Strategies Involving Mass Spectrometry for the Determination of Composition and Structure of Oligosaccharides Derived from Glycoproteins* **Perreault H.**, Saba J.A., Kunkel J., Williams T.T.L., Jamieson J.C.

10:20 Coffee Break

10:40 0016 *Single Molecule Enzymology* **Craig D.B.**

11:00 0017 *Small is Beautiful: Analytical Chemistry in Microfluidic Devices.* **Skinner C.D.**

11:20 End of Session

Biological & Medicinal

BM4 La Salle

Protein Engineering

Organizer - J. Keillor
Chair - J.W. Keillor

08:15 Introductory Remarks

08:20 0018 *Directed Evolution to Enhance Enantioselectivity of a Pseudomonas fluorescens Esterase Using a Fast, Accurate Screening Method* **Horsman G.P.**, Liu A.M.F., Kazlauskas R.J.

08:40 0019 *Novel Heterodimeric Coiled-Coil Peptide Pairs Selected in Vivo from a designed Library-vs-Library Ensemble* **Pelletier J.N.**, Arndt K.M., Müeller K.M., Plückthun A., Michnick S.W., Alber T.

09:00 0020 *Photo-control of Peptides and Coiled-Coils by a Modified Azobenzene "Conformational Switch"* Kumita J.R., Flint D.G., Smart O.S., **Woolley G.A.**

09:20 0021 *Quantitative mapping of biochemical pathways in living cells* **Michnick S.**

09:40 0022 *Design of Protein Catalysts* **Hilvert D.**

10:20 Coffee Break

10:40 0023 *A Perspective On Biological Catalysis* **Benkovic S.J.**

11:20 End of Session

BM6 Westmount

Recent Advances in Drug Discovery

Organizer - M. Bös & C. Yoakim
Chair - C. Yoakim

Antivirals

08:55 Introductory Remarks

09:00 0024 *A Structural Basis for Understanding Drug-Resistance Mutations in HIV Reverse Transcriptase.* Huang H., Chopra R., Harrison S., **Verdine G.L.**

INDEX of Authors

The name of each author is followed by the Abstract Number and the Symposium Code. As in the Main Program, presenting authors are designated in bold text.

43 09:40 Sunday IN8 Outremont

Condensation and Characterization of Metal Chalcogenolate Clusters inside Mesoporous MCM-41 C.M. Kowalchuk, J.F. Corrigan and Y. Huang, Department of Chemistry, The University of Western Ontario, London, Ontario, N6A 5B7.

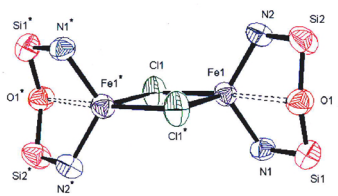
The impregnation of MCM-41 with metal chalcogenolate clusters has recently been demonstrated.[1,2] The structural integrity of these clusters once inside the mesopores has been investigated through ^{31}P MAS NMR, UV-vis and Raman spectroscopies. Loss of the phosphine ligands provides a unique opportunity for examining modified cluster molecules in a stable mesoporous environment. Cluster modification may be promoted through thermal or photochemical means. Controlled thermolysis of $Cu_6(TePh)_6(PEtPh_2)_5$ proceeds through ejection of five $PEtPh_2$ and six $TePh_2$ moieties with copper telluride remaining in the MCM-41 pores which is described through PXRD and TEM measurements. Photochemical irradiation results in loss of $TePh_2$ and condensation in one dimension of larger cluster species due to the spatial confinement of MCM-41 as examined by TEM and UV-vis spectroscopy. Our recent results in these areas will be presented.

1. C. M. Kowalchuk, Y. Huang, J. F. Corrigan, Chem. Commun., **2000**, 1811-1812.
2. C. M. Kowalchuk, Y. Huang, J. F. Corrigan, Stud. Surf. Sci. Catal., **2000**, 129 (Nanoporous Materials II, Proceedings of the Conference on Access in nanoproous Materials, 2000).

44 10:00 Sunday IN8 Outremont

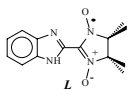
Spin-Admixed and Intermediate Spin Iron(III) Diamidoether Complexes G. Mund, P.H. Bhatia, R.J. Batchelor and D.B. Leznoff, Simon Fraser University, Department of Chemistry, Burnaby B.C. V5A 1S6.

The majority of iron(III) compounds are found to be in either the high-spin (n=5 unpaired electrons) or low-spin state (n=1). A small number of macrocyclic complexes show intermediate-spin (n=3) or quantum spin-admixed magnetic behaviour. We are investigating these unusual spin states of iron(III) in non-macrocyclic systems. The reaction of FeX_3 (X=Cl, Br) with $Li_2\{[^tBuN(SiMe_2)]_2O\}$ ($[^{tBu}NON]$) gives a compound of empirical formula $[^{tBu}NON]FeCl$. The X-ray crystal structure reveals this compound to be a dimer with chloride bridges (see figure; ^{t}Bu and Me groups removed for clarity). This compound displays spin-admixed (S = 5/2, 3/2) behaviour, rare for a non-macrocyclic Fe(III) compound. Replacement of the t-butyl groups with 2,4,6-Me_3Ph moieties generates a complex with a pure S = 3/2 state. Introduction of the highly steric 2,6-iPr_2Ph groups further influences the magnetic properties of the system. These unusual Fe(III) spin-states have been explored using variable temperature magnetic susceptibility, ESR and Mossbauer spectroscopies and their UV-vis data, which shifts as a function of spin-state, will also be reviewed. The analogous bromide complexes have also been prepared in order to examine the effect of changing halide on the magnetic properites of this system.



45 10:40 Sunday IN8 Outremont

Unprecedented Magnetic and Optical Properties of New Nitroxyde Coordination Complexes with Rare Earth Ions C. Lescop, D. Luneau and P. Rey, Laboratoire de Reconnaissance Ionique et Matériaux Moléculaires, C.E.A. Grenoble, DRFMC, SCIB, RI2M, UMR 5046, 17, Rue des Martyrs, F38054 Grenoble Cedex 09, FRANCE; G. Bussière, M. Triestre and C. Reber, Équipe FCAR de Chimie Inorganique, Université de Montréal, Montréal, QC, H3C 3J7, CANADA.



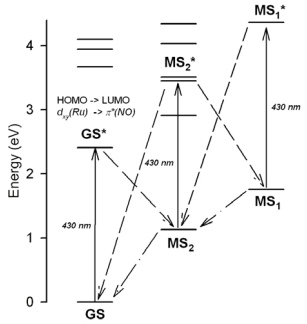
In this contribution, we will report the syntheses, crystal structures, magnetic behaviours and optical properties of a family of rare earth metal ions M (M = La^{III}, Eu^{III} and Gd^{III}) coordination complexes with nitronyl - nitroxyde radicals L substituted with benzimidazolyl moities. Additionnally, the first complexes of rare earth metal ions with imino-nitroxyde radicals L' (benzimidazolyl substituted) and L'' (2-pyridinyl substitted) are presented. Complexes with stoechiometries ML_4, ML_2, ML_1, ML'_1 and ML''_1 have been characterised. Unprecedented antiferromagnetic interactions[1] between rare earth ion and radical are observed for ML_4, ML_2, ML'_1, ML''_1 while ML1 exhibits a classical ferromagnetic interaction. In order to get information about the magnetic interaction pathway that could explain such unexpected results, the optical properties of this family of complexes have been investigated down to 5 K. A ligand centred luminescence phenomenon[2] has been observed for the complexes of nitronyl-nitroxyde radicals while with the Eu^{III} complexes, a competition occurs between this ligand centered luminescence and the classical Eu^{III} centered luminescence. On the basis of these experiments, a new model to explain the magnetic pathway interaction between rare earth metal ions and radical ions is presented.

[1] : Lescop, C., Luneau, D., Belorizky, E., Fries, P., Guillot, M., Rey,P., Inorg. Chem., 1999, 38, 5472.
[2] : Lescop, C., Luneau, D., Bussière, G., Triest, M., Reber, C., Inorg. Chem, 2000, 39(17), 3740-3741.

46 11:00 Sunday IN8 Outremont

Properties of Metastable States of Ruthenium Nitrosyl Complexes. DFT and TD-DFT Study S.I. Gorelsky and A.B.P. Lever, Department of Chemistry, York University,, 4700 Keele St., Toronto, ON M3J1P3.

Recently, much attention has been focused on studies of the metastable states of transition metal nitrosyl complexes and predominantly on the nitroprusside ion.
We studied the properties of the $[R(NH_3)_5NO]^{3+}$ and $[Ru(CN)_5NO]^{2-}$ ions using density functional theory (DFT). The electronic ground-state potential surface of these nitrosyl complexes has two local minima (metastable states) with oxygen (MS_1) bonded NO, i.e. inverted from the usual N-bonded species (GS), and with NO which is bound sideways (MS_2). While thermochemical and spectroscopic properties of the $[Ru(CN)_5NO]^{2-}$ ion resemble closely those of the nitroprusside ion, the corresponding properties of the $[Ru(NH_3)_5NO]^{3+}$ ion are rather different. In $[Ru(CN)_5NO]^{2-}$ and $[Fe(CN)_5NO]^{2-}$ ions, the MS_2 state lies 1.1-1.4 eV above the GS state and 0.3-0.6 eV below the MS_1 state, but in the $[Ru(NH_3)_5NO]^{3+}$ ion, the MS_2 state is slightly above the MS_1. In the visible region, the electronic spectrum of ruthenium nitrosyl complexes contains MLCT bands, $4d\pi(Ru) \rightarrow e(\pi^*\ NO)$. Using time-dependent DFT (TD-DFT) calculations it is possible to explain why the MS_2 state of $[Ru(NH_3)_5NO]^{3+}$ has not been observed experimentally.



47 08:20 Sunday MA3 Mount Royal

Design and Utility of Sulfur-Nitrogen-Phosphorus Polymers For Sensing Applications I. Manners, Department of Chemistry,, University of Toronto,, Toronto, Ontario, Canada, M5S-3H6.

In collaboration with the group of Mitch Winnik we have been exploring the use of inorganic polymers for the construction of phosphorescent sensors. In this talk the development of polythionylphosphazenes for applications such as the measurement of pressure distributions over aircraft and automobiles in wind tunnels and dissolved oxygen in ground water will be discussed.[1,2]

1. McWilliams, Gates, Edwards, Liable-Sands, Guzei, Rheingold, Manners, *J. Am. Chem. Soc.* **2000** p 8848.
2. Ruffolo, Evans, Lu, Winnik, Manners et *al. Analytical Chem.* **2000** p 1894.

48 09:00 Sunday MA3 Mount Royal

A New Class of Lanthanide Chelates for Biomedical Imaging D.J. Bornhop, S. Robertson, T. Goebel and J.M.M. Griffin, Department of Chemistry and Biochemistry, Southwest Cancer Center, Texas Tech University; G. Kiefer, Dow Chemical, Freeport Texas; D. Morgan, Department of Pathology, Texas Tech University Health Sciences Center; B. Bell and M. Motamedi, Center for Biomedical Engineering, University of Texas Medical Branch, Galveston, TX 77555.

A new class of exogenous marker, based on polyazamacrocycic chelates of Tb (III) or Eu (III) that are non-toxic, have good water solubility and exhibit attractive spectral properties, will be shown to be useful for biomedical fluorescence imaging. Synthesis, as well as the physical, chemical, spectroscopic and physiological properties for these unique chemical markers will be discussed. It will also be shown that their use for quantitative minimally invasive tissue imaging is possible at endoscopy. Furthermore, it will be shown that one of these chelates, Tb-PCTMB, {Tb-3,6,9-tris(methylene phosphonic acid n-butyl ester)-3,6,9,15-tetraaza-bicyclo[9.3.1]pentadeca-1(15),11,13-triene} shows a preference to bind abnormal tissue allowing the potential for enhanced disease detection. For example, DMH-induced colon cancer in the Sprague Dawley Rat can be detected (specificity of 86% and sensitivity of 94%) using low concentration topical doses of Tb-PCTMB, low power excitation and visual detection. Enhanced detection of the polyazamacrocycic lanthanide chelates using time-resolved imaging has been possible and will be discussed as an alternate in-vivo imaging modality.

Inorganic

IN7 La Salle

Solid State Chemistry

Organizer - A. Mar
Chair - I. Davidson

13:35		Introductory Remarks
13:40	0647	*Rationalizing and Predicting Simple Crystal Topologies* **Lee S.**
14:20	0648	*Extended Metal Dibenzoylmethanates, a New Class of Host Materials* **Soldatov D.V.**

14:40	0649	*Intrazeolite Organometallic Kinetics: Annealing & Decarbonylation Studies of $Mo(CO)_6$ in $Na_{56}Y$ and Temperature Dependence of Reactions of $Mo(CO)_6$ with Chemisorbed PMe_3 in $Na_{56}Y$* Fernandez A.L., Hao J., Poe A.J., **Teeple R.L.**, Vichi E.J.S.
15:00		Coffee Break
15:20	0650	*Polyferrocenylsilane and Magnetic Ceramic Microspheres* **Kulbaba K.**, Resendes R., Cheng A., Bartole A., Safa-Sefat A., Coombs N., Stover D.H., Greedan J.E., Ozin G.A., Manners I.
15:40	0651	*Synthesis and Electronic Properties of Potassium Fulleride Nanowires in a Mesoporous Niobium Oxide Host* **Ye B.**, Trudeau M., Antonelli D.

16:00	0652	*Mapping out the Connectivities in Intermediate Gel Phases of Molecular Sieve Synthesis by Solid-State NMR* **Huang Y.**, Machado D., Richer R.
16:20	0653	*Solid State NMR Studies of Battery Materials and Ionic Conductors* , Lee Y.J., Paik Y., Kim N., Chaudhuri S.**Grey C.P.**
17:00		End of Session

Database Statistics (9/14/2001)

```
================================================================================
General Statistics
================================================================================
1224 : Number of Abstracts
1027 : Number of Scheduled Abstracts
 197 : Number of Unscheduled Abstracts
1250 : Highest Abstract Number
   0 : Number of Withdrawn Abstracts
  22 : Number of Unnotified Abstracts
  18 : Number of Damaged Abstracts
 335 : Number of Abstracts with Graphics
--------------------------------------------------------------------------------
List of Unused Abstract ID's
   2,   53,   58,   67,   83,  106,  127,  200,  225,  297,  315,  432
,  463,  489,  545,  562,  563,  705,  711,  759,  808, 1004, 1129, 12
17, 1228, 1234
--------------------------------------------------------------------------------
List of Abstract's whose symposium or division is unassigned
  97,  104,  271,  300,  364,  470,  507,  707,  904,  984, 1065, 1066
, 1072, 1115, 1191, 1250
================================================================================
Abstract Counts By Symposium (empty symposia omitted)
Total  Sched  UnSched
================================================================================
Unassigned Division
--------------------------------------------------------------------------------
  16 :    0 :   16 : Unassigned Symposium
================================================================================
Analytical
--------------------------------------------------------------------------------
  23 :    9 :   14 : Spectroscopy and Imaging of Surfaces (Including Electrodes)
  18 :   13 :    5 : Advances in Engineering of Biosensors for Biomedical Applications
  40 :   26 :   14 : Analysis of Biomolecules, Drugs and Metabolites
   8 :    4 :    4 : Higher Throughput Analytical Techniques
  11 :   10 :    1 : Use of Lasers in Analytical Chemistry
  15 :    8 :    7 : Electrochemistry
   7 :    7 :    0 : NEWs in Analytical Chemistry
   2 :    0 :    2 : Sensor Development for Environmental Analysis (Joint with Environmental)
  11 :   11 :    0 : Combinatorial Chemistry: Synthesis and Analysis (Joint with Organic)
  10 :    9 :    1 : New Methods for Analysis of Persistent Organic Pollutants (Joint with Environ
================================================================================
Biological & Medicinal
--------------------------------------------------------------------------------
   7 :    7 :    0 : Advances in the Analysis & Structure Determination of Biomolecules
   4 :    4 :    0 : Intellectual Property & Chemistry
  22 :   22 :    0 : Bioorganic Chemistry
   6 :    6 :    0 : Protein Engineering
  11 :   11 :    0 : Molecular Diversity (Joint with Organic)
  13 :   13 :    0 : Recent Advances in Drug Discovery
  11 :   11 :    0 : Medicinal Chemistry of Nucleosides & Nucleic Acids; in Honour of Professor Ke
   8 :    8 :    0 : General Session
================================================================================
Chemical Education/College Chemistry Canada
--------------------------------------------------------------------------------
   3 :    3 :    0 : History of the Pharmaceutical Industry in Canada (Joint with Biological & Med
  10 :   10 :    0 : Chemistry Teaching Laboratories for the New Millenium: Changes and Challenges
   9 :    9 :    0 : How do I do it ? - Experiments and Demonstrations for Introductory Chemistry
   5 :    5 :    0 : Teaching Chemistry to Non-Chemistry Students and Explaining it to the General
  10 :   10 :    0 : Role of the TA in Chemistry Teaching
   8 :    8 :    0 : General Session
   8 :    8 :    0 : Poster Session and Exam Question Exchange
================================================================================
Environmental
--------------------------------------------------------------------------------
   7 :    7 :    0 : Air Quality Issues
   8 :    8 :    0 : Effluent Treatment and Solids Management
   1 :    0 :    1 : Sensor Development for Environmental Analysis (Joint with Analytical)
================================================================================
```

Inorganic

5	0	5	Materials for Use in Electronics and Photonics (Joint with Macromolcular)
13	11	2	Multifunctional Lewis Acids (Joint with Organic)
14	14	0	Unusual Structure and Bonding for the p - Block Elements
15	15	0	Bioinorganic and Inorganic Medicinal Chemistry
20	17	3	Fluorine Chemistry (Joint with Organic)
18	16	2	Ruthenium Chemistry in Catalysis and Organic Synthesis, (a Symposium Honoring
24	24	0	Solid State Chemistry
66	48	18	General Session

Macromolecular Sciences & Engineering

20	20	0	Polymers for Pharmaceutical Applications
17	17	0	Functional and Controlled Architecture Polymers
40	40	0	Materials for Use in Electronics and Photonics (Joint with Inorganic)
33	33	0	General Session

Organic

28	19	9	Organic Reactions and Processes
24	24	0	Organic Synthesis using Organometallic Reagents
18	16	2	Heterocycles
2	0	2	Combinatorial Chemistry: Synthesis and Analysis (Joint with Analytical)
8	8	0	Synthesis and Recognition in Carbohydrate Chemistry, A Symposium in Memory of
15	14	1	Mechanistic Aspects of Electron Transfer in Organic Chemistry
29	19	10	General session

Physical & Theoretical

39	0	39	History and Applications of Theoretical Chemistry (Joint with Chemical Educat
15	15	0	Advances in Spectromicroscopy
9	9	0	Scanning Probe Microscopy of Biosurfaces
11	11	0	Materials Research Using Synchrotron Radiation (Joint with Materials)

Analytical

13	0	13	Poster Session

Biological & Medicinal

71	70	1	Poster Session

Environmental

13	13	0	Poster Session

Inorganic

103	87	16	Poster Session

Macromolecular Sciences & Engineering

40	40	0	Poster Session

Organic

119	119	0	Poster Session

Physical & Theoretical

45	39	6	Poster Session

CIC/CSC Awards

1	0	1	CIC Medal
1	0	1	Montréal Medal
1	1	0	Union Carbide Award
1	0	1	Macromolecular Science and Engineering Award

Plenary Lecture

1	1	0	Plenary Lecture

Analytical			
5	5	0	Award Lectures
Environmental			
9	9	0	General Session
Physical & Theoretical			
6	6	0	General Session
1224	1027	197	Totals